

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 321 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.01e-01

Confidence level: 6.23e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Ethyl phthalyl ethyl glycolate</div> <div>Measured: 347</div> <div>Predicted: 319</div>	<div>Image not found</div> <div>Thiophanate-methyl</div> <div>Measured: 1780</div> <div>Predicted: 864</div>	<div>Image not found</div> <div>Crotoxyphos</div> <div>Measured: 100</div> <div>Predicted: 123</div>
<div>Image not found</div> <div>Benomyl</div> <div>Measured: 513</div> <div>Predicted: 354</div>	<div>Image not found</div> <div>Oxycarboxin</div> <div>Measured: 95.5</div> <div>Predicted: 175</div>	